

On selection criteria for problems with moving inhomogeneities

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Abstract

We study mechanical problems with multiple solutions and introduce a thermodynamic framework to formulate two different selection criteria in terms of macroscopic energy productions and fluxes. Simple examples for lattice motion are then studied to compare the implications for both resting and moving inhomogeneities.

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1 Introduction

Many equations describing mechanical systems exhibit more than one solution, and a common problem is then to select physically reasonable solutions. The central aim of the paper is to analyse selection conditions for problems with inhomogeneities, such as sources or phase interfaces.

In the literature one finds three commonly cited selection criteria. Two of them are reminiscent of Sommerfeld, who gives two physical reasonings of his *radiation condition* for standing sources [Som49, Som62]. He first states that sources have to be sources, and then stipulates that energy cannot flow in from infinity. The third selection criterion is the *causality principle* introduced by Slepian [Sle01, Appendix A], see also the monograph [Sle02], which determines the admissible group speeds on both sides of the inhomogeneity. All these criteria have been applied mainly in the context of Fourier analysis.

In this paper, we present a different approach to selection criteria, based on thermodynamic fields, which are derived via hyperbolic scaling limits and Young measures and describe the underlying mechanical systems on large spatial and temporal scales. In particular, we show that Sommerfeld's two formulations of his radiation condition are naturally related to rather different fields such as *production of oscillatory energy* and *radiation flux*. Our framework covers arbitrary nonlinear Hamiltonian lattices and PDEs, but we have to specialise to linear or almost linear cases in order to obtain explicit expressions for the thermodynamic fields.

While we recover Sommerfeld's results for standing sources, the case of a moving phase interface turns out to be remarkably different. Specifically, in the first case we find that both thermodynamic selection criteria are equivalent and agree with the causality principle. In the second case, however, the condition on radiation (energy) fluxes can be in contradiction to the entropy inequality, the production criterion and the causality principle. Thus the energy flux criterion should not be applied uncritically to problems with moving inhomogeneities.

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We present our exposition along two guiding examples of nearest neighbour (NN) chains of atoms. The governing equations are

$$\ddot{x}_j(t) = \Phi'(x_{j+1}(t) - x_j(t)) - \Phi'(x_j(t) - x_{j-1}(t)) + \zeta(t)\delta_{j0}, \quad (1)$$

where ζ is the external forcing of atom $j = 0$, and the two examples are (i) a harmonic chain with periodic forcing ζ , (ii) a moving phase interface in a chain with bi-quadratic interaction potential Φ and no external forcing.

Sommerfeld's radiation condition Sommerfeld's approach to radiation conditions is described in his book [Som62, §28], see also [Som49], and we thus just describe the gist of some key arguments. However, the discussion given in §3 for the case of a lattice model closely resembles the original spatially continuous case, and we refer the reader to that section for a more detailed mathematical treatment.

Sommerfeld considers the wave equation on \mathbb{R}^3 with a temporally periodic forcing at the origin. A separation of variables ansatz leads to the Helmholtz equation with a source at the origin, thus an inhomogeneous equation. The corresponding homogeneous equation has nontrivial bounded kernel functions (in \mathbb{R}^3). Some kernel functions are excluded by boundary or symmetry conditions, in Sommerfeld's case by requiring that the solution is radially symmetric and decaying at infinity. This still does not single out a unique solution. In particular, there are two singular and decaying solutions u^\pm to the inhomogeneous Helmholtz equation, which are well-defined outside the origin. Let x^\pm be the corresponding solutions of the forced wave equation. The choice of the direction of time made in the separation of variables *ansatz* renders the corresponding solution x^+ an *outwardly* radiating radial wave and x^- an *inwardly* radiating wave. In fact, x^+ describes a *source* solution to the forced wave equation in the sense that the forcing supplies energy to the system. On the contrary, x^- corresponds to a sink solution, as the forcing now deprives the system of energy.

Sommerfeld now introduces a *binary* choice, allowing only waves which propagate outwards and dismissing those which propagate inwards. This selection is necessary both for physical and mathematical reasons: mathematically, the choice is an integral part of the arguments leading to a unique fundamental solution of the forced wave equation. Physically the two solutions x^\pm are qualitatively very different. In Sommerfeld's words [Som62],

$$\text{"Quellen sollen *Quellen*, nicht Senken der Energie sein." [Sources have to be sources, not sinks of the energy.]} \quad (\text{SOM1})$$

We call this the *first formulation* of Sommerfeld's radiation condition. He then gives what we call the *second formulation*,

$$\text{"Die von den Quellen ausgestrahlte Energie mu\ss sich ins Unendliche zerstreuen, Energie darf nicht aus dem Unendlichen in die vorgeschriebenen Singularit\aten des Feldes eingestrahlt werden." [The energy radiated from the sources has to scatter to infinity, energy must not be radiating from infinity into the prescribed singularities of the field.]} \quad (\text{SOM2})$$

Thermodynamic approach In §2 we establish a thermodynamic framework to analyse (SOM1) and (SOM2). The starting point are *discrete local conservation laws*, which can be derived from (1) and describe the transport of mass, momentum and energy on the *microscopic scale*. In a first step we introduce a small scaling parameter ε and use the concept of *Young measures* to establish the macroscopic limit $\varepsilon \rightarrow 0$. In this limit the microscopic conservation laws converge to their macroscopic counterparts, which are PDEs with densities, fluxes and productions.

In a second step we identify the macroscopic quantities that admit a thermodynamic interpretation of Sommerfeld's radiation condition. The *radiation flux* Q is defined as the Galilean invariant part of the energy flux and (SOM1) is naturally related to the sign of Q on both sides of the inhomogeneity. We also introduce the *oscillatory energy* E_{osc} , which measures the amount of macroscopic energy stored in microscopic oscillations, and the *non-oscillatory energy* E_{non} . Sommerfeld's first formulation

of the radiation condition can now be reinterpreted in terms of energy productions. More precisely, for forced excitation problems as studied by Sommerfeld for the wave equation, (SOM1) is naturally related to the sign of the local production of total energy $E = E_{\text{osc}} + E_{\text{non}}$ due to the external forcing. The situation is different for phase transition waves as these are not driven by external forces and conserve the total energy exactly (in a local sense). Instead, the key energetic phenomenon is now that the propagating phase interface causes a constant transfer between oscillatory and non-oscillatory energy. This transfer gives rise to a production of oscillatory energy, and (SOM1) is naturally related to the sign of this production.

Notice that the above arguments are solely based on energy productions and fluxes, that means on fundamental concepts from continuum mechanics and thermodynamics. They can therefore, at least in principle, be also applied to more general systems, as for instance NN chains with generic double-well potentials. However, only in some special cases it is also possible to derive *explicit* expressions for all densities, fluxes and production terms.

We finally emphasise that our macroscopic interpretations of (SOM1) and (SOM2) provide only *necessary* conditions. To ensure uniqueness, in particular to exclude linear combinations of x^+ and x^- in Sommerfeld's forced excitation problem, one typically imposes *microscopic selection criteria*, which also exploit non-macroscopic properties of solutions. Examples are the asymptotic radiation condition (21) or, equivalently, the causality principle. Both methods are inextricably connected with Fourier methods. It is therefore not clear how to generalise these selection criteria to nonlinear problems.

Results for the special examples In §3 we apply the thermodynamic framework to the analogue of Sommerfeld's problem in the harmonic NN chain and find that (SOM1) and (SOM2) are equivalent and comply with the microscopic selection criterion. Afterwards we study phase transition waves in §4 and show that both conditions provide different selection criteria for moving phase interfaces. We show that (SOM1) is equivalent to the usual entropy inequality, and thus we propose to apply (SOM1) to problems with moving inhomogeneities as well. The application of (SOM2), however, turns out to be problematic. Specifically, we show that for subsonic wave speed close to the speed of sound, the selection criterion (SOM2) selects a phase transition wave that *violates* the entropy inequality as well as the causality principle. We thus conclude that (SOM2) has to be discarded, at least for some problems with moving inhomogeneities.

2 Macroscopic field equations in the presence of microscopic oscillations

Our approach to Sommerfeld's radiation condition in §3 and §4 is based on macroscopic balance laws that govern the effective dynamics of averaged quantities on large spatial and temporal scales. In this section we derive and discuss these balance laws and provide the atomistic expressions for all densities, fluxes and production terms. Our exposition is formal but we emphasise that all arguments can be made rigorous using Young measures; see [DH08, DHR06] and Appendix A. For the sake of clarity, we start with the conservation laws for the unforced NN chain, that is (1) with $\zeta = 0$.

Microscopic conservation laws We can rewrite (1) with $\zeta = 0$ in terms of the atomic distances (discrete strains) $r_j := x_{j+1} - x_j$, and velocities $v_j := \dot{x}_j$ as first order equations

$$\dot{r}_j = v_{j+1} - v_j, \quad \dot{v}_j = \Phi'(r_j) - \Phi'(r_{j-1}), \quad (2)$$

which can be viewed as the discrete counterparts of the local conservation laws for mass and momentum in Lagrangian coordinates, see (6). We note that (2) constitute *local conservation laws* in the sense that the time derivate of some atomistic observable equals the discrete divergence of another observable. As a consequence we find, assuming appropriate decay conditions for $j \rightarrow \pm\infty$, that each local conservation law implies a global one by summing over j . The discrete divergence structure is also an important

ingredient for the thermodynamic limit because it allows us to derive the macroscopic conservation laws, see Appendix A.

Since the unforced NN chain is an autonomous Hamiltonian system with shift symmetry, we can also derive a local conservation law for the energy, namely

$$\frac{d}{dt} \left(\frac{1}{2} v_j^2 + \Phi(r_{j-1}) \right) = v_j \Phi'(r_j) - v_{j-1} \Phi'(r_{j-1}). \quad (3)$$

To characterise the thermodynamic properties of NN chains, we now derive a macroscopic description by applying the *hyperbolic scaling* of space and time. For a given scaling parameter $0 < \varepsilon \ll 1$, we define the *macroscopic time* τ and the *macroscopic particle index* ξ by

$$\tau = \varepsilon t, \quad \xi = \varepsilon j, \quad (4)$$

but we do *not* scale distances and velocities. We then regard the atomistic data that correspond to a solution of (2) as functions r_ε and v_ε that depend continuously on τ and are piecewise constant in ξ . That is, we identify $r_j(t) = r_\varepsilon(\varepsilon t, \varepsilon j)$ and $v_j(t) = v_\varepsilon(\varepsilon t, \varepsilon j)$.

Of course, the functions r_ε and v_ε will, in general, be highly oscillatory with wave length of order ε and do not converge as $\varepsilon \rightarrow 0$ in a pointwise sense. However, as long as the solution to (2) is *bounded* we can assume, thanks to weak compactness, that for any *atomic observable* $\psi = \psi(r, v)$ the functions $\psi(r_\varepsilon, v_\varepsilon)$ converge weakly as $\varepsilon \rightarrow 0$, see Appendix A. The limit function $\langle \psi \rangle$ is then non-oscillatory and can be regarded as the *thermodynamic field* of ψ , which means that $\langle \psi \rangle(\tau, \xi)$ gives the local mean value of ψ in the macroscopic point (τ, ξ) .

Macroscopic conservation laws In the thermodynamic limit $\varepsilon \rightarrow 0$ the discrete conservation laws (2) and (3) transform into

$$\partial_\tau \langle r \rangle = \partial_\xi \langle v \rangle, \quad \partial_\tau \langle v \rangle = \partial_\xi \langle \Phi'(r) \rangle, \quad \partial_\tau \langle \frac{1}{2} v^2 + \Phi(r) \rangle = \partial_\xi \langle v \Phi'(r) \rangle. \quad (5)$$

These PDEs describe the local conservation laws for mass, momentum and energy on the macroscopic scale and are well known within the thermodynamic theory of elastic bodies. In fact, they can be written as

$$\partial_\tau R - \partial_\xi V = 0, \quad \partial_\tau V + \partial_\xi P = 0, \quad \partial_\tau E + \partial_\xi F = 0, \quad (6)$$

with *macroscopic strain* $R = \langle r \rangle$, *macroscopic velocity* $V = \langle v \rangle$, *pressure* $P = -\langle \Phi'(r) \rangle$, *total energy density* $E = \langle \frac{1}{2} v^2 + \Phi(r) \rangle$, and *total energy flux* $F = -\langle v \Phi'(r) \rangle$. Moreover, splitting off the Galilean invariant part from both the energy density and the energy flux, we find

$$E = \frac{1}{2} V^2 + U, \quad F = V P + Q, \quad (7)$$

with *internal energy density* U and heat flux Q . *Radiation* in the sense of Sommerfeld precisely means energy transport via Q , see also §3, and therefore we call Q the *radiation flux*.

We emphasise that, in general, the conservation laws (6) do *not* constitute a closed system, but must be accompanied by *closure relations*. Unfortunately, very little is known about the thermodynamic limit for most initial data and general interaction potentials. In some cases, however, it is possible to solve the closure problem. Below we show that all thermodynamic fields can be computed explicitly for (i) Sommerfeld's fundamental solution in forced harmonic NN chains and (ii) phase transition waves in NN chains with bi-quadratic potential.

Oscillatory energy For our purposes, the split (7) is not sufficient; it is convenient to introduce another split of the total energy density E that accounts for the fact that the computations of local mean values and nonlinearities do not commute in the presence of oscillations. To obtain a precise measure for the strength of the oscillations we write

$$E = E_{\text{non}} + E_{\text{osc}}, \quad E_{\text{non}} = \frac{1}{2} V^2 + \Phi(R),$$

which means

$$E_{\text{non}} = \frac{1}{2}\langle v \rangle^2 + \Phi(\langle r \rangle), \quad E_{\text{osc}} = \frac{1}{2}\langle (v - \langle v \rangle)^2 \rangle + \langle \Phi(r) - \Phi(\langle r \rangle) \rangle \quad (8)$$

and furthermore implies $U = \Phi(\langle r \rangle) + E_{\text{osc}}$. We refer to E_{osc} and E_{non} as oscillatory and non-oscillatory energy density, respectively, and emphasise that E_{osc} measures precisely the amount of macroscopic energy that is locally stored within the oscillations. From (5) and (8) we now conclude that the partial energies are balanced by

$$\partial_\tau E_{\text{osc}} + \partial_\xi Q = \Xi, \quad \partial_\tau E_{\text{non}} + \partial_\xi(PV) = -\Xi, \quad (9)$$

where the production terms are given by

$$\Xi = -(P + \Phi'(R))\partial_\xi V = (\langle \Phi'(r) \rangle - \Phi'(\langle r \rangle))\partial_\xi \langle v \rangle.$$

The physical meaning of Ξ becomes apparent when we compute the temporal change of the oscillatory and non-oscillatory energy contained in a control volume $\Omega = [a, b]$. This gives

$$\frac{d}{d\tau} \int_a^b E_{\text{osc}} d\xi + Q|_{\xi=a}^{\xi=b} = \int_a^b \Xi d\xi = -\frac{d}{d\tau} \int_a^b E_{\text{non}} d\xi - (PV)|_{\xi=a}^{\xi=b}.$$

Since the flux terms Q and PV are related to the exchange of energy with the exterior of Ω , we conclude that $\Xi(t, \xi)$ measures precisely how much non-oscillatory energy is transferred into oscillatory energy at time τ at the point ξ .

We further mention that the second law of thermodynamics is, at least on an intuitive level, related to a sign condition for Ξ . While each scaling limit of the unforced NN chain conserves the total energy according to (5)₃, there exist many solutions that yield a non-vanishing field Ξ in the limit $\varepsilon \rightarrow 0$. For $\Xi \geq 0$ these solutions ‘dissipate’ non-oscillatory energy (at the expense of increasing oscillatory energy); this is in perfect agreement with our physical intuition since oscillations can be regarded as microscopic fluctuations. If time is reversed, however, Ξ becomes negative and the solution extracts energy from the fluctuations, which contradicts the intuition. This is discussed in more detail in §3 and §4.

Thermodynamic fields for harmonic oscillations With the central quantities E_{osc} and E_{non} now being defined, we can return to the analysis of thermodynamic fields. Motivated by the discussion in §3 and §4, we restrict the analysis and compute the thermodynamic fields for *travelling waves* in harmonic NN chains. A travelling wave for the NN chain is an exact solution to (1) with $\zeta = 0$ that satisfies

$$r_j(t) = \mathcal{R}(j - c_{\text{ph}}t), \quad v_j(t) = \mathcal{V}(j - c_{\text{ph}}t) \quad (10)$$

for some *phase speed* c_{ph} and *profile functions* \mathcal{R} and \mathcal{V} that depend on the phase variable $\varphi = j - c_{\text{ph}}t$. Travelling waves in NN chains are determined by advance-delay differential equations, see [FV99, DHM06, Her10], and describe fundamental *oscillatory patterns*.

The hyperbolic scaling (4) implies that each travelling wave solution for the harmonic NN chain (10) converges as $\varepsilon \rightarrow 0$ to a Young measure that is constant in space and time. The thermodynamic fields of all observables ψ are therefore independent of (τ, ξ) and can be computed from R and V as follows

$$\langle \psi \rangle := \lim_{L \rightarrow \infty} \frac{1}{2L} \int_{-L}^L \psi(\mathcal{R}(\varphi), \mathcal{V}(\varphi)) d\varphi. \quad (11)$$

For a harmonic NN chain, which has the interaction potential $\Phi(r) = \frac{1}{2}c_0^2 r^2 + d_1 r + d_0$, we immediately verify by Fourier transform that for prescribed c_{ph} with $0 < |c_{\text{ph}}| < c_0$ travelling waves are

given by

$$\mathcal{R}(\varphi) = R + \sum_{i=1}^M A_i \cos(\kappa_i \varphi + \kappa_i/2 + \eta_i), \quad \mathcal{V}(\varphi) = V \mp c_0 \sum_{i=1}^M A_i \cos(\kappa_i \varphi + \eta_i), \quad (12)$$

with “−” and “+” for left and right moving waves, respectively, that is, for $c_{\text{ph}} < 0$ and $c_{\text{ph}} > 0$, respectively. Here the wave numbers κ_i , $i = 1, \dots, M$, denote the positive solutions to $c_{\text{ph}}^2 k^2 = \Omega(k)^2$, where $\Omega(k) = 2c_0 \sin(k/2)$ is the dispersion relation of the harmonic NN chain. In particular, near sonic waves with $c_{\text{ph}} \approx c_0$ have $M = 1$ and depend, up to the phase shift η_1 , on the four independent parameters R , V , $A = A_1$, and $\kappa = \kappa_1$.

The thermodynamic fields for such harmonic travelling waves can easily be computed by (11) and (12). In fact, thanks to $\langle r \rangle = R$ and $\langle v \rangle = V$, we find

$$P = -c_0^2 R - d_1, \quad E_{\text{non}} = \frac{1}{2} V^2 + \frac{1}{2} c_0^2 R^2 + d_1 R + d_0, \quad (13)$$

as well as

$$E_{\text{osc}} = \frac{1}{2} c_0^2 A^2, \quad Q = \pm \left(c_0 \sum_{i=1}^M \frac{A_i}{A} \cos(\kappa_i/2) \right) E_{\text{osc}} \quad (14)$$

with $A^2 = \sum_{i=1}^M A_i^2$. For periodic waves with $M = 1$ we therefore have $Q = c_{\text{gr}} E_{\text{osc}}$, where $c_{\text{gr}} = \pm |\Omega'(\kappa)|$ is the *group speed*.

We emphasise that the thermodynamic computations presented above can be extended to superpositions of finitely many harmonic travelling waves, with obvious modifications. We also mention that a complete characterisation of the energy transport in harmonic lattices can be derived in terms of Wigner-Husimi measures [Mie06].

Macroscopic description of forcing In order to generalise the formalism from above to forced NN chains we assume, for simplicity, that the forcing acts only in the particle $j = 0$, see (1), and that ζ is periodic with

$$\zeta(t) = \zeta(t + t_{\text{per}}), \quad \int_0^{t_{\text{per}}} \zeta(t) dt = 0. \quad (15)$$

These conditions guarantee that the forcing does not contribute to the macroscopic conservation laws for mass, $(2)_1$, and momentum, $(2)_2$. The forcing, however, in general supplies some energy to the system, and hence the conservation law $(2)_3$ must be replaced by

$$\partial_\tau E + \partial_\xi F = \theta(\tau) \delta_0(d\xi). \quad (16)$$

The *macroscopic energy production* at $\xi = 0$ can be computed either as the jump of the macroscopic energy flux at $\xi = 0$ or by averaging the microscopic energy production. This reads

$$\theta(\tau) = F(\tau, 0+) - F(\tau, 0-) = \lim_{\delta \rightarrow 0} \lim_{\varepsilon \rightarrow 0} \frac{\varepsilon}{2\delta} \int_{(\tau-\delta)/\varepsilon}^{(\tau+\delta)/\varepsilon} v_0(t) \zeta(t) dt. \quad (17)$$

3 The forced harmonic NN chain

Here we present the analogue to Sommerfeld’s classical problem in harmonic NN chains, that is, the localised forced excitation problem

$$(\partial_t^2 - c_0^2 \Delta_1) x_j(t) = \zeta(t) \delta_j^0, \quad (18)$$

where Δ_1 denotes the discrete Laplacian $\Delta_1 x_j := x_{j+1} + x_{j-1} - 2x_j$. For simplicity we normalise the speed of sound to $c_0 = 1$ and assume that the chain is periodically forced at one of its eigenfrequencies σ with $0 < \sigma < 2$. The analysis presented in this section resembles that of the spatially continuous case studied by Sommerfeld [Som62]; the purpose of this section is to familiarise readers with our approach to selection criteria, and to show that we recover Sommerfeld's classical results for a standing source in a spatially discrete medium.

Explicit solutions via Helmholtz equation The separation of variables *ansatz* $x_j(t) = \text{Re}(u_j \exp(-i\sigma t))$ transforms (18) into the discrete Helmholtz equation

$$\sigma^2 u_j + \Delta_1 u_j = \delta_0, \quad (19)$$

which can be solved by Fourier transform. There exist two *special solutions* u^+ and u^- defined by

$$u_j^\pm = \pm \frac{\exp(\pm i\kappa |j|)}{i2\Omega(\kappa)\Omega'(\kappa)},$$

where $\kappa = \kappa(\sigma)$ denotes the unique solution to

$$\sigma^2 = \Omega(k)^2, \quad \Omega(k) = 2 \sin(k/2), \quad 0 < k < \pi.$$

Of course, the special solutions u^- and u^+ can be linearly combined and also superimposed by plane waves with wave numbers $\pm\kappa$, which are the kernel functions of the discrete Helmholtz operator. The general solution to (19) can therefore be parameterised by $\alpha, \beta \in \mathbb{C}$ as

$$u_j = u_j(\alpha, \beta) = u_j^+ + \alpha \exp(-i\kappa j) + \beta \exp(+i\kappa j). \quad (20)$$

Note that in particular $u_j^+ = u_j(0, 0)$ and $u_j^- = u_j(\alpha^-, \beta^-)$ with $\alpha^- = \beta^- = -(i2\Omega(\kappa)\Omega'(\kappa))^{-1}$.

Sommerfeld's approach to the radiation condition can be viewed as the endeavour to remove the non-uniqueness and to single out a unique choice for α and β . To this end, he introduces a microscopic selection criterion, whose analogue in the harmonic NN chains reads

$$\lim_{j \rightarrow +\infty} \left(\frac{du_j}{dj} - i\kappa u_j \right) = 0, \quad \lim_{j \rightarrow -\infty} \left(\frac{du_j}{dj} + i\kappa u_j \right) = 0, \quad (21)$$

and implies that $\alpha = \beta = 0$ in (20). In particular, the microscopic radiation condition selects u^+ but rules out u^- .

Macroscopic aspects of Sommerfeld's radiation condition We now show that the binary choice between u^- and u^+ can be understood in terms of purely macroscopic conditions on the production of oscillatory energy and the direction of the radiation fluxes. As remarked in §2, the thermodynamic framework can be extended to superpositions of harmonic waves. It is thus possible to characterise all bounded solutions to (18), in particular kernel functions and their superpositions. The result of such an analysis is that the thermodynamic interpretation of (SOM1) and (SOM2) rejects superpositions of waves as long as their influx contribution exceeds the outward contribution. Thus, a half space of all bounded solutions is rejected, and a half-space accepted. We show this analysis here in detail for the two extreme cases corresponding to u_- and u_+ . The analysis for the other solutions is, *mutatis mutandis*, analogous yet more complicated terms arise.

At first we notice that u^+ and u^- correspond to the real-valued displacements

$$x_j^\pm(t) = \frac{\sin(\kappa |j| \mp \sigma t)}{2\Omega(\kappa)\Omega'(\kappa)}.$$

Each of these solutions to (18) consists of two counter-propagating travelling waves that are glued together at $j = 0$, where the travelling waves propagate towards and away from the inhomogeneity at

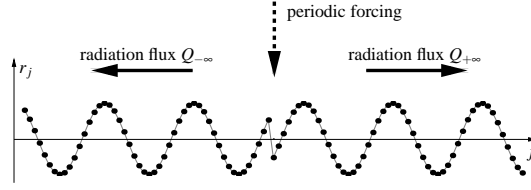


Figure 1: Sommerfeld's *source solution* for the harmonic NN chain: The energy pumped in by the periodic forcing is radiated towards both $+\infty$ and $-\infty$. If time is reversed the source becomes a sink and the radiation fluxes on both sides change their sign.

$j = 0$ for x^+ and x^- , respectively. We also notice that x^+ and x^- transform into each other under time reversal, and that they define the atomic distances and velocities

$$v_j^\pm(t) = \mp A \cos(\kappa |j| \mp \sigma t), \quad r_j^\pm(t) = A \cos(\kappa |j + \frac{1}{2}| \mp \sigma t) \quad (22)$$

where the amplitude $A > 0$ is given by $1/A = 2\Omega'(\kappa) = 2 \cos(\kappa/2)$.

To determine the thermodynamic limit $\varepsilon \rightarrow 0$, the key observation is that both x^- and x_+ generate Young measures that are (i) independent of the macroscopic time $\tau = \varepsilon t$, (ii) constant for $\xi < 0$ and $\xi > 0$, where $\xi = \varepsilon j$ is the macroscopic particle index, and (iii) generated by periodic travelling waves. These assertions follow directly from (22) and the definition of Young measure convergence, see §2 and Appendix A. They also imply that the macroscopic conservation laws (6) are trivially satisfied for $\xi \neq 0$. The relevant macroscopic information is therefore encoded in jump conditions for the thermodynamic fields at $\xi = 0$.

Using (13) and (14) we now conclude that almost all thermodynamic fields are globally constant with

$$R = 0, \quad V = 0, \quad P = 0, \quad F = Q, \quad E_{\text{non}} = 0, \quad E = E_{\text{osc}}, \quad E_{\text{osc}} = \frac{1}{2}A^2,$$

while the radiation flux Q is piecewise constant, $Q(\tau, \xi) = \pm \text{sign}(\xi) \Omega'(\kappa) E_{\text{osc}} =: Q_{\text{sgn}(\xi)\infty}$. The two values for Q are given by

$$Q_{-\infty} = \mp \frac{1}{4}A, \quad Q_{+\infty} = \pm \frac{1}{4}A,$$

and computing the macroscopic energy production by averaging, see (17), we find

$$\theta = -\frac{\sigma}{2\pi} \int_0^{2\pi/\sigma} v_0(t) \cos(\sigma t) dt = \pm \frac{\sigma A}{2\pi} \int_0^{2\pi/\sigma} \cos(\sigma t)^2 dt = \pm \frac{1}{2}A.$$

Sommerfeld's first condition (SOM1) is naturally related to the sign of θ . For x^+ we have $\theta > 0$, so the forcing pumps in energy at $j = 0$ and the solution describes a *source* of the energy. The solution x^- , however, corresponds to a *sink* as $\theta < 0$ implies that energy flows out constantly at $j = 0$. Moreover, for the solutions at hand the balance of total energy reduces to

$$\theta = Q_{+\infty} - Q_{-\infty} = 2Q_{+\infty} = -2Q_{-\infty},$$

and implies that Sommerfeld's first and second formulation of the radiation condition are equivalent. Namely, energy that is pumped in at $j = 0$ must be radiated away, and hence the radiation fluxes must point away from $j = 0$, see Fig. 1. Conversely, energy that is deprived from the system at $\xi = 0$ must be radiated in from $\pm\infty$. We thus conclude that both (SOM1) and (SOM2) select the solution x^+ but reject x^- .

We close this section by mentioning that the *causality principle*, see [Sle01, Sle02] and the discussion in §4, requires that all oscillatory modes in front and behind the interface satisfy $c_{\text{gr}} > c_{\text{ph}}$ and $c_{\text{gr}} < c_{\text{ph}}$, respectively. It is not hard to see that this principle also favours x^+ and, more generally, implies (SOM2) for a standing source.

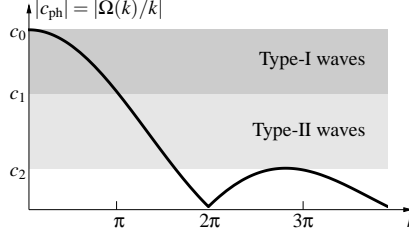


Figure 2: Phase transition waves with $|c_{\text{ph}}| > c_2$ have periodic tails and come in two different types. Type-I waves have either $0 < c_{\text{gr}} < c_{\text{ph}}$ or $0 > c_{\text{gr}} > c_{\text{ph}}$, whereas type-II waves correspond to either $c_{\text{gr}} < 0 < c_{\text{ph}}$ or $c_{\text{gr}} > 0 > c_{\text{ph}}$.

4 Phase transition waves for a bi-quadratic NN chain

We now consider travelling waves with a moving inhomogeneity and apply the selection criteria (SOM1) and (SOM2) to these waves. We mention, however, two important caveats of our analysis: firstly, we assume the existence of subsonic travelling waves with a single inhomogeneity (interface). Guidance for the existence can be taken from [TV05]; yet existence is a subtle issue, and a rigorous existence proof is available only for a small regime of subsonic velocities [SZ09, SZ]; it is also worth mentioning that there is a velocity regime where no travelling waves with a single interface can exist [SSZ]. Secondly, the selection criteria that result from the thermodynamic interpretation of (SOM1) and (SOM2) are *necessary* but not sufficient.

We now study heteroclinic solutions to the travelling wave equation (10). To calculate the thermodynamic fluxes explicitly, we restrict our considerations to the NN chain with piecewise quadratic interaction potential

$$\Phi(r) = \frac{1}{2} \min \left\{ (r-1)^2, (r+1)^2 \right\}, \quad (23)$$

but mention that our thermodynamic arguments can, at least in principle, be generalised to genuinely nonlinear potentials as well. (The double-well nature of Φ describes the co-existence of different stable states and thus the possibility of interfaces between those states.)

The potential (23) is normalised to have unit sound speed, $c_0 = 1$. As illustrated in Figure 2, there is a critical velocity $c_2 > 0$ such that for all with c_{ph} with $c_2 < |c_{\text{ph}}| < 1$ there is a unique solution $\kappa > 0$ to

$$c_{\text{ph}}^2 k^2 = \Omega^2(k), \quad \Omega(k) = 2 \sin(k/2). \quad (24)$$

From now on we solely consider waves with $|c_{\text{ph}}| > c_2$ because then the tails are periodic with a unique wave number κ as chosen above. This means, for any travelling wave with a single interface we have

$$(\mathcal{R}, \mathcal{V})(\varphi) \xrightarrow{\varphi \rightarrow \pm\infty} (\mathcal{R}_{\pm\infty}, \mathcal{V}_{\pm\infty})(\varphi), \quad (25)$$

where both $(\mathcal{R}_{+\infty}, \mathcal{V}_{+\infty})$ and $(\mathcal{R}_{-\infty}, \mathcal{V}_{-\infty})$ are periodic travelling waves (possibly constant) with phase speed c_{ph} and group speed c_{gr} . To compute the thermodynamic fields explicitly, it is necessary that the asymptotic microscopic strains are confined to the harmonic wells. We thus require that both $\mathcal{R}_{-\infty}$ and $\mathcal{R}_{+\infty}$ have a definite sign. By symmetry we can assume that $\mathcal{R}_{\pm\infty}(\varphi) \gtrless 0$, and by shift invariance we can also assume that $\mathcal{R}(0) = 0$. Thus, the interface moves along $j = c_{\text{ph}}t$ and $\xi = c_{\text{ph}}\tau$ in the microscopic and macroscopic space-time coordinates, respectively. Notice, however, that we have not fixed the sign of c_{ph} , so the wave travels from negative strain to positive strain for $c_{\text{ph}} > 0$, and the other way around for $c_{\text{ph}} < 0$.

Macroscopic constraints for phase transition waves Under the assumption that travelling waves with a single interface as described above exist, all thermodynamic fields are constant on the

left and on the right of the interface and are completely determined by the periodic tail oscillations in (25). The macroscopic conservation laws therefore reduce to jump conditions via $\partial_\tau \rightsquigarrow -c_{\text{ph}} \llbracket \cdot \rrbracket$ and $\partial_\xi \rightsquigarrow \llbracket \cdot \rrbracket$, so the PDEs (6) transform into

$$c_{\text{ph}} \llbracket R \rrbracket = -\llbracket V \rrbracket, \quad c_{\text{ph}} \llbracket V \rrbracket = \llbracket P \rrbracket, \quad c_{\text{ph}} \llbracket E_{\text{non}} + E_{\text{osc}} \rrbracket = \llbracket PV + Q \rrbracket. \quad (26)$$

Note that the asymptotic jump and mean value of any thermodynamic field X are given by

$$\llbracket X \rrbracket = X_{+\infty} - X_{-\infty}, \quad \{X\} = \frac{1}{2}(X_{+\infty} + X_{-\infty}), \quad X_{\pm\infty} = \lim_{\xi \rightarrow \pm\infty} X(\tau, \xi).$$

We now express the asymptotic values of all thermodynamic fields X in terms of $R_{\pm\infty}$, $V_{\pm\infty}$, $A_{\pm\infty}$, and the speeds c_{ph} and c_{gr} . In this way, we recover well-known jump conditions and kinetic relations for phase transition waves [Tru82, Tru93]. The strategy of computing thermodynamic quantities as averages of atomic observables is well established, see for instance [TV05, SCC05]. However, it is usually not based on Young measures and hyperbolic scaling limits. It further seems that the concepts of oscillatory and non-oscillatory energy have not been used before in the context of phase transition waves.

Due to (23) and the sign choice for $\mathcal{R}_{\pm\infty}$, we have $P_{\pm\infty} = -\Phi'(R_{\pm\infty}) = -R_{\pm\infty} \pm 1$ and hence $\llbracket P \rrbracket = 2 - \llbracket R \rrbracket$. The jump conditions for mass (26)₁ and momentum (26)₂ thus imply

$$\llbracket R \rrbracket = \frac{2}{1 - c_{\text{ph}}^2}, \quad \llbracket V \rrbracket = -\frac{2c_{\text{ph}}}{1 - c_{\text{ph}}^2}, \quad (27)$$

and therefore

$$\llbracket E_{\text{non}} \rrbracket = 2 \frac{c_{\text{ph}}^2 \{R\} - c_{\text{ph}} \{V\}}{1 - c_{\text{ph}}^2}, \quad \llbracket PV \rrbracket = 2 \frac{c_{\text{ph}} \{R\} - c_{\text{ph}}^2 \{V\}}{1 - c_{\text{ph}}^2}.$$

Using this and the formulae for E_{osc} and Q from (14), we then find

$$-c_{\text{ph}} \llbracket E_{\text{non}} \rrbracket + \llbracket PV \rrbracket = 2c_{\text{ph}} \{R\}, \quad -c_{\text{ph}} \llbracket E_{\text{osc}} \rrbracket + \llbracket Q \rrbracket = (c_{\text{gr}} - c_{\text{ph}}) \llbracket E_{\text{osc}} \rrbracket, \quad (28)$$

which is the analogue to (9). Consequently, the jump condition for the total energy (26)₃ enforces that the productions for oscillatory and non-oscillatory energy cancel via

$$\Xi = -2c_{\text{ph}} \{R\} = (c_{\text{gr}} - c_{\text{ph}}) \llbracket E_{\text{osc}} \rrbracket. \quad (29)$$

This formula is important as it reveals that for phase transition waves there is no production of total energy but instead a steady transfer between the oscillatory and the non-oscillatory contributions of the energy. This transfer has power $-2\{R\}$ and drives the wave. More precisely, the *configurational force* Υ satisfies

$$c_{\text{ph}} \Upsilon = \Xi, \quad \Upsilon := \llbracket \Phi(R) \rrbracket - \{\Phi'(R)\} \llbracket R \rrbracket.$$

This is the *kinetic relation* and follows from (27) and (28) thanks to $\llbracket E_{\text{non}} \rrbracket = \llbracket V \rrbracket \{V\} + \llbracket \Phi(R) \rrbracket$, $\llbracket PV \rrbracket = \{P\} \llbracket V \rrbracket + \llbracket P \rrbracket \{V\}$ and $P = -\Phi'(R)$. The production of oscillatory energy Ξ is the process commonly called dissipation. Recall, however, that the total energy $E = E_{\text{osc}} + E_{\text{non}}$ is not dissipated but conserved according to the energy laws (6)₃ and (26)₃.

We finally notice that time reversal changes the sign of c_{ph} , c_{gr} , Ξ , $V_{\pm\infty}$, $Q_{\pm\infty}$, but does not affect $R_{\pm\infty}$, $A_{\pm\infty}$, $E_{\text{osc}, \pm\infty}$, $E_{\text{non}, \pm\infty}$, $P_{\pm\infty}$, or Υ . We also observe that all thermodynamic fields are completely determined by

$$c_{\text{ph}}, \quad A_{-\infty}, \quad A_{+\infty}, \quad \{V\}. \quad (30)$$

In fact, from (30) we compute κ and c_{gr} by (24) and set $\llbracket E_{\text{osc}} \rrbracket = \frac{1}{2} \llbracket A^2 \rrbracket$. Afterwards we solve (27)₁ and (29) for $R_{-\infty}$ and $R_{+\infty}$, which then allow us to compute $V_{-\infty}$ and $V_{+\infty}$ from (27)₂.

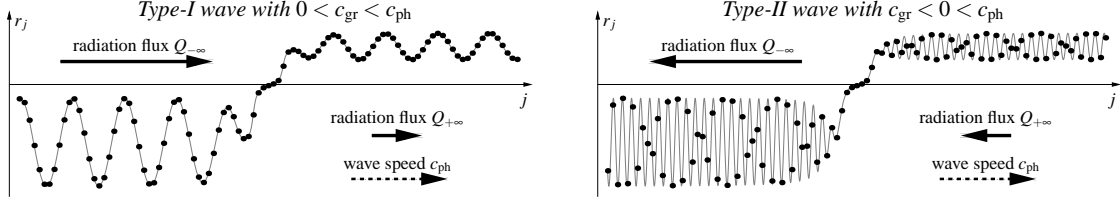


Figure 3: Phase transition waves are driven by a constant transfer between the oscillatory and the non-oscillatory energy and the radiation fluxes on both sides of the interface have the same sign. The cartoons illustrate the *source* solutions for type-I and type-II waves, which represent different order relation for the group velocity c_{gr} and the phase velocity c_{ph} . If time is reversed, the interface becomes a sink of oscillatory energy and the radiation fluxes on both sides change their sign.

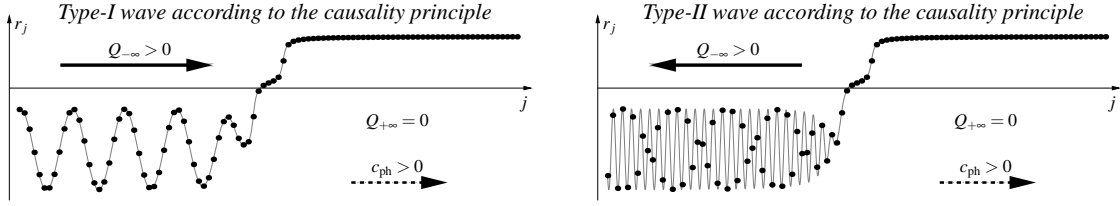


Figure 4: The causality principle selects phase transition waves that propagate into a region without oscillations. These waves are, up to Galilean invariance, uniquely determined by their speed c_{ph} .

The jump conditions derived in this section constitute *macroscopic constraints* which are *necessary* for the existence of a phase transition wave with speed $|c_{\text{ph}}| \in (c_2, 1)$. However, it was proven in [SZ] that these conditions are also *sufficient*, at least for near sonic speeds with $0 < 1 - |c_{\text{ph}}| \ll 1$. In conclusion, there exists a four-parameter family of candidates for phase transition waves, that means of heteroclinic travelling waves. It is now very natural to ask which of them are physically reasonable, and so selection criteria come into play.

The macroscopic aspects of Sommerfeld’s radiation conditions We first consider (SOM1). It is reasonable to require that the interface is a source rather than a sink of oscillatory energy. The production Ξ therefore has to be non-negative, which means

$$\Xi = (c_{\text{gr}} - c_{\text{ph}})[E_{\text{osc}}] \geq 0. \quad (31)$$

This inequality is *equivalent* to

$$c_{\text{ph}} \Upsilon \geq 0, \quad (32)$$

which is the usual *entropy condition* for phase transition waves (see for example [TV05]). For all waves considered here, (31) implies $E_{\text{osc}, +\infty} < E_{\text{osc}, -\infty}$ for waves moving to the right and $E_{\text{osc}, +\infty} > E_{\text{osc}, -\infty}$ for left-moving waves. In other words, in all cases we have $\Xi > 0$ if and only if the oscillations have smaller amplitude in front of the interface than behind the interface. (SOM1) select these solutions but rejects waves that travel from regions of low oscillations into regions of high oscillations. Note, however, that oscillations in front of the interface are not ruled out since it is only required that the wave propagates in direction of decreasing oscillations. This implies that there is still a four-parameter family of phase transition waves which satisfy (SOM1).

Sommerfeld’s second formulation (SOM2), which stipulates that “energy is carried away from the interface”, translates directly into a condition on the radiation flux. It requires, on both sides of the interface, that Q points away from the interface. This condition is very restrictive for phase transition waves with periodic tails because both $Q_{-\infty}$ and $Q_{+\infty}$ have the same sign as the group velocity c_{gr} ,

see (14). Thus (SOM2) can only be satisfied if there are no oscillations on one side of the interface. However, which side of the interface is chosen by (SOM2) depends on the sign of c_{gr} , and therefore we distinguish between two types, see Figures 2 and 3. Type-I waves have $c_1 < |c_{\text{ph}}| < 1$, where $c_1 := 2\Omega(\pi/2)/\pi$, and this implies $\text{sgn } c_{\text{gr}} = \text{sgn } c_{\text{ph}}$ and $|c_{\text{gr}}| < |c_{\text{ph}}|$. Type-II waves correspond to $c_2 < |c_{\text{ph}}| < c_1$, which means $\text{sgn } c_{\text{gr}} \neq \text{sgn } c_{\text{ph}}$.

For type-I waves, the radiation fluxes behind and in front of the interface point towards and away from the interface, respectively. This is illustrated in Figure 3, and holds regardless whether (31) is satisfied or not. Energy is therefore always radiated towards the interface, and the second formulation of the radiation condition can only be satisfied if there are no oscillations behind the interface. Those waves, however, are usually regarded as unphysical as they violate (31) and (32). The only solution candidates that would be accepted by both formulations have no oscillations, neither in front nor behind the interface; however, such single transition waves do not exist for the potential (23).

The discussion is different for type-II waves. There is still radiation into the interface but now the radiation flux impinges from ahead of the interface. Therefore, both (SOM1) and (SOM2) are simultaneously satisfied by type-II waves that propagate into a region without oscillations, that is, $E_{\text{osc}, +\infty} = 0$ for right-moving waves and $E_{\text{osc}, -\infty} = 0$ for left-moving waves. In particular, there exists a three-parameter family of type-II waves that satisfy both (SOM1) and (SOM2).

In summary, for type-I waves, and hence for near sonic waves, (SOM1) and (SOM2) contradict each other and would, if applied together, reject any bounded phase transition wave with a single interface. For type-II waves, however, (SOM2) implies (SOM1) and allows for a three-parameter family of waves. This is in stark contrast to the case of a standing source discussed in §3, where both criteria are equivalent.

Microscopic selection criteria Besides macroscopic criteria as described above, there also exist microscopic selection principles for phase transition waves. These are far more restrictive and select a two-parameter family of phase transition waves, as shown below. For the sake of comparison we now summarise the main arguments leading to microscopic selection criteria for phase transition waves in bi-quadratic NN chains and refer to [TV05, CCS05] for more details. The key idea is that under the condition $\text{sgn } \mathcal{R}(\varphi) = \text{sgn } \varphi$, each phase transition wave is determined by the affine advance-delay-differential equation

$$c_{\text{ph}}^2 \partial_\varphi^2 \mathcal{R} = \Delta \mathcal{R} - \Delta \text{sgn } \varphi.$$

This equation can be regarded as the analogue to the inhomogeneous Helmholtz equation (19), and solutions can be represented by $\mathcal{R}(\varphi) = \text{Re}(\mathcal{S}(\varphi))$ with

$$\mathcal{S}(\varphi) = -\frac{i}{\pi} \int_{\Gamma} \frac{\Omega(k)^2 \exp(+ik\varphi)}{k\Omega^2(k) - c_{\text{ph}}^2 k^3} dk, \quad (33)$$

where Γ is an appropriately chosen contour in the complex plane. The microscopic selection criterion is based on the *causality principle* [Sle01, Sle02] and requires that all oscillatory modes in front and behind the interface satisfy $c_{\text{gr}} > c_{\text{ph}}$ and $c_{\text{gr}} < c_{\text{ph}}$, respectively. The contour Γ is therefore chosen as the dented real axis that passes the origin $k = 0$ from below but the other real-valued poles of the integrand in (33) from above. Jordan's lemma from complex-valued calculus then provides the following expressions for the thermodynamic fields for a right moving wave

$$R_{\pm\infty} = \pm \frac{c_{\text{ph}}}{1 - c_{\text{ph}}^2} + \frac{c_{\text{ph}}}{c_{\text{gr}} - c_{\text{ph}}}, \quad A_{-\infty} = \frac{2c_{\text{ph}}}{c_{\text{gr}} - c_{\text{ph}}}, \quad A_{+\infty} = 0, \quad (34)$$

with $[V]$ as in (27), and therefore

$$[E_{\text{osc}}] = -\frac{2c_{\text{ph}}^2}{(c_{\text{gr}} - c_{\text{ph}})^2} < 0, \quad \Xi = \frac{2c_{\text{ph}}^2}{c_{\text{ph}} - c_{\text{gr}}} > 0. \quad (35)$$

In particular, there exists a two-dimensional family of phase transition waves that is parameterised by the speed c_{ph} and the trivial parameter $\{V\}$. All these causality waves have no oscillations ahead of the interface and (SOM1) is always satisfied. The validity of (SOM2), however, depends on $\text{sgn } c_{\text{gr}} = \text{sgn } Q$, i.e., on whether the wave is of type-I or type-II. This is illustrated by the two cartoons from Figure 4. We therefore find again that (SOM2) has different implications for the two wave types. This is not surprising since a condition on the sign of $c_{\text{ph}} - c_{\text{gr}}$ does not imply any constraint for $\text{sgn } c_{\text{gr}} = \text{sgn } Q$, or *vice versa*. In other words, (SOM2) does not imply the causality principle, or *vice versa*. For a type-I wave the causality principle even implies that energy is radiated towards the interface from behind, see the left panel in Figure 4.

We recall that for standing sources as discussed in §3, the causality principle in fact implies (SOM2). It is therefore tempting to adopt the criterion (SOM2) for moving phase interfaces and reformulate this condition as “the energy flux has to point away from the interface, with reference to an observer travelling with the interface”. Let us follow this argument for causality waves as shown in Figure 4. Changing to the co-moving frame via $\tilde{j} = j - c_{\text{ph}}t$ and $\tilde{\xi} = \xi - c_{\text{ph}}\tau$, the partial energy balances (9) transform into

$$\partial_{\tau}E_{\text{osc}} + \partial_{\tilde{\xi}}(Q - c_{\text{ph}}E_{\text{osc}}) = +\Xi, \quad \partial_{\tau}E_{\text{non}} + \partial_{\tilde{\xi}}(PV - c_{\text{ph}}E_{\text{non}}) = -\Xi.$$

In view of $Q = c_{\text{gr}}E_{\text{osc}}$ we now conclude that the causality principle implies that the *relative radiation flux* $\tilde{Q} = Q - c_{\text{ph}}E_{\text{osc}}$ has the same sign as $\tilde{\xi}$, and is hence indeed pointing away from the interface on both sides. The flaw with this argument, however, is that the passage to the co-moving frame is not a Galilei transformation since both j and ξ are Lagrangian space coordinates (Galilei transformations are given by $u_j \mapsto u_j + ct$). The observation that \tilde{Q} has a certain sign on both sides of the interface does therefore not imply that the interface radiates energy towards infinity. The correct treatment is to work with the Lagrangian space coordinates j and ξ and to characterise the radiative parts of the energy flux in terms of Q . This flux can, as shown in Figure 4, point towards the interface from the tail of the wave.

Selection rules from Riemann problems A different approach to microscopic selection criteria is via initial values problems. The main idea is to characterise the physically relevant solutions as the limit as $t \rightarrow \infty$ of reasonable initial data. For the NN chains with double well potential, a rigorous mathematical analysis of initial values problems is not yet available, but numerical simulations provide a lot of insight into the implied selection criteria.

To illustrate this, we now present two numerical solutions of initial value problems for the NN chain with interaction potential (23). Due to the Hamiltonian nature of (1), we perform the simulations with the Verlet scheme (see, e.g., [HLW02] for details), which is a symplectic integrator and does not add numerical viscosity to the problem. In order to enforce the formation of macroscopic waves, we start with Riemann initial data, that means we set

$$r_j(0) = r_{\pm\infty}, \quad v_j(0) = v_{\pm\infty} \quad \text{for} \quad j \gtrless 0,$$

with prescribed asymptotic data $r_{\pm\infty}$, $v_{\pm\infty}$. Moreover, we choose a ‘number of particles’ $N \gg 1$ and introduce the scaling parameter $\varepsilon = 1/N$. We then integrate the lattice equation on the domain $|j| \leq N/2$ over the time interval $0 \leq \tilde{t}_{\text{fin}}N$ with $0 < \tilde{t}_{\text{fin}} < 1/2$. To this end we close the discrete equations (2) by imposing Dirichlet boundary data for r and v . Notice that the choice of the computational domain and time is in accordance with both the hyperbolic scaling and $c_0 = 1$, this means no macroscopic wave can hit the boundary of the computational domain.

Figures 5 and 6 depict the numerical results at time \tilde{t}_{fin} for two Riemann problems with $\text{sgn}(r_{-\infty}) \neq \text{sgn}(r_{+\infty})$. The left panel contains snapshots of the atomic distances against the scaled particle index $\tilde{j} = \varepsilon j$, and the other panels show the spatial profiles of macroscopic strain R and heat flux Q , which are computed by mesoscopic averaging; see [DH08] for details.

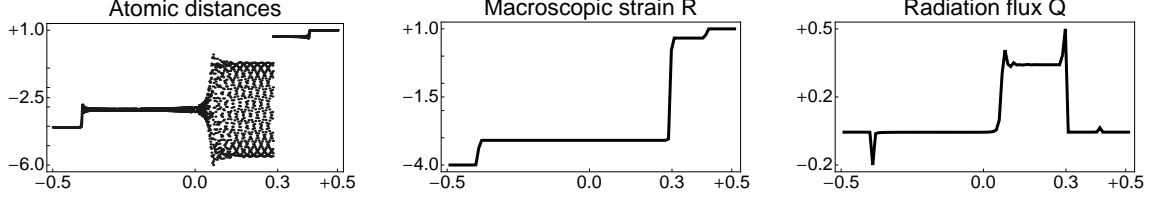


Figure 5: Numerical solutions to the Riemann problem with $r_{-\infty} = -4$, $r_{+\infty} = +1$, $v_{-\infty} = +1$, $v_{+\infty} = -1$ and $N = 4000$, $\bar{t}_{\text{fin}} = 0.4$. The microscopic dynamics selects a type-I wave satisfying the causality principle.

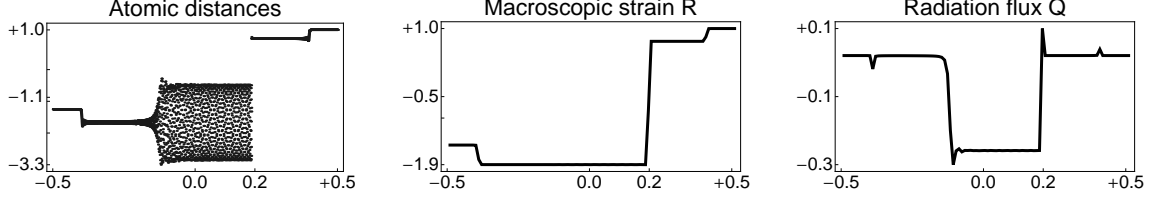


Figure 6: Numerical solutions to the Riemann problem with $r_{-\infty} = -3/2$, $r_{+\infty} = +1$, $v_{-\infty} = +1$, $v_{+\infty} = -1$ and $N = 4000$, $\bar{t}_{\text{fin}} = 0.4$. The microscopic dynamics selects a type-II wave satisfying the causality principle.

In both simulations we observe four elementary waves connecting five constant states. Starting from the left side we find: Left initial state, first wave, first non-oscillatory intermediate state, second wave, oscillatory intermediate state, third wave, second non-oscillatory intermediate state, fourth wave, and the right initial state. The first and the fourth wave, which both connect two non-oscillatory states, are contact discontinuities and correspond to jumps in the linear wave equation. The second wave, which connects to the oscillatory intermediate state, is still a harmonic phenomenon since the oscillations are confined to one of the quadratic wells of Φ . We also notice that the macroscopic strain does not change within the second wave.

The third wave, however, describes a phase transition as it connects negative strain to positive strain. A closer look to the oscillatory intermediate state reveals that it is generated by a single harmonic travelling wave which has a certain phase velocity c_{ph} . The third wave propagates with the same speed c_{ph} , and hence it corresponds in fact to a heteroclinic travelling wave in the lattice. We finally mention that for $\varepsilon > 0$ we still have harmonic fluctuations within the constant intermediate state and near the contact discontinuities, but these disappear in the thermodynamic limit $\varepsilon \rightarrow 0$.

Figures 5 and 6 reveal that the radiation flux Q within the oscillatory intermediate state has a different sign in both simulations. More precisely, we see a type-I wave in Figure 5 but a type-II wave in Figure 6. Recall that both waves are now ‘chosen’ by the microscopic dynamics (more precisely, by the numerical scheme). In other words, the macroscopic structure of the Riemann solution (the parameters of the waves and the intermediate states) determine — implicitly, but nevertheless uniquely — a microscopic selection rule for phase transition waves. We are not able to derive this selection rule rigorously from the lattice dynamics although this should, in principle, be possible. However, computing the speed of the interface as well as thermodynamic fields on both sides of the interface, we find that these meet very well the predictions from the causality principle described above, see (34) and (35). It would be highly desirable to understand this in greater detail and to find a reformulation of the causality principle that can also be applied to generic double well potentials, where Fourier methods can no longer be used. First steps into this direction are already done in this paper, because our thermodynamic approach to radiation conditions can be generalised to more complicate nonlinear problems. However, we emphasise that many questions remain open.

Discussion The discussion in this section shows that the case of a moving interface is different from that of a standing source; for the latter, (SOM1) and (SOM2) are equivalent. For moving interfaces in phase transition waves we find that (SOM1), which is formulated in terms of sources and sinks, is equivalent to the entropy condition (32). The flux condition (SOM2), however, implies (SOM1) for type-II waves but both rules contradict each other for type-I waves.

For moving interfaces, one has therefore to distinguish between arguments that rely on the energy transport in terms of fluxes, as (SOM2), and arguments based on energy productions, as (SOM1). Since (SOM1) is equivalent to the entropy inequality, we propose to apply this selection criterion for moving inhomogeneities. We also propose that flux based criteria such as (SOM2) should *not* be naïvely applied to problems with moving inhomogeneities.

These suggestions are in line with the causality principle used in [Sle01, Sle02, TV05] and numerical simulations of Riemann-type problems for NN chains.

A Appendix: Macroscopic conservation laws for NN chains

We establish the thermodynamic limit for the forced NN chain (1) provided that the forcing ζ satisfies (15). Our goal is to show that the macroscopic balance laws for mass, momentum and energy (see (5) and (16)) can be derived rigorously as follows:

1. The hyperbolic scaling transforms each *bounded* solution into a family of *oscillatory* functions which depend on the macroscopic time τ and macroscopic Lagrangian space coordinate ξ .
2. This family of functions is compact in the sense of Young measures, and hence we can extract convergent subsequences. Along such a subsequence, the limit measure encodes the *local distribution functions* of the oscillatory data and hence the *local mean values* of atomic observables. These local mean values provide the *thermodynamic fields* and are, by construction, *non-oscillatory* functions in τ and ξ .
3. The dynamics of NN chains implies that the thermodynamic fields of each Young measure limit satisfy the macroscopic conservation laws of mass, momentum and energy (in a distributional sense).

We now collect the mathematical tools for each of these steps. We start with some basic facts about Young measures and refer the reader to [Bal89, Rou97, Val94, Tay97] for more details.

Let Ω be a domain in \mathbb{R}^k and K be some convex and closed set in \mathbb{R}^m . A Young measure $\mu \in Y(\Omega; K)$ is a Ω -family of probability measures on K , that means a measurable map $\mu: y \in \Omega \rightarrow \mu(y, dQ) \in \text{Prob}(K)$. Notice that each function $Q: \Omega \rightarrow K$ defines a trivial Young measure with $\mu(y, dQ) = \delta_{Q(y)}(dQ)$, where $\delta_{Q(y)}(dQ)$ abbreviates the delta distribution in $Q(y)$.

Theorem 1 (Fundamental Theorem on Young Measures). *Each family*

$$(Q_\varepsilon)_{0 < \varepsilon \leq 1} \subset L^\infty(\Omega; K)$$

is compact in the space of Young-measures $YM(\Omega; K)$. This means there exists a sequence $(\varepsilon_n)_{n \in \mathbb{N}}$ with $\varepsilon_n \rightarrow 0$ along with a limit measure $\mu \in YM(\Omega; K)$ such that

$$\psi(Q_{\varepsilon_n}) \xrightarrow{n \rightarrow \infty} \langle \psi \rangle \quad \text{weakly}^* \text{ in } L^\infty(\Omega) \quad (36)$$

for all observables $\psi \in C(K)$, where

$$\langle \psi \rangle(y) = \int_B \psi(Q) \mu(y, dQ)$$

gives the local mean value of ψ in $y \in \Omega$.

Proof. See, for instance, [Tay97], Proposition 11.3 in Section 13.11. \square

The convergence (36) is equivalent to

$$\int_{\Omega} \langle \psi \rangle(y) \phi(y) dy = \lim_{n \rightarrow \infty} \int_{\Omega} \psi(Q_{\varepsilon_n}(y)) \phi(y) dy \quad (37)$$

for all test functions $\phi \in C_c^\infty(\Omega)$. Moreover, the subsequence converges strongly to some limit function Q_0 in $L^\infty(\Omega; K)$ if and only if the limit measure is trivial, $\mu(y, dQ) = \delta_{Q_0(y)}(dQ)$.

We now suppose that we are given a bounded solution to (1). As in §2, we regard the atomic distances $r_j = u_{j+1} - u_j$ and velocities $v_j = \dot{u}_j$ as the basic variables, i.e., we consider

$$Q_j(t) = (r_j(t), v_j(t)), \quad j \in \mathbb{Z}, \quad t \geq 0. \quad (38)$$

For a given scaling parameter $0 < \varepsilon \leq 1$ we introduce τ and ξ by (4), so the macroscopic Lagrangian space-time coordinate is given by

$$\Omega = \{(\tau, \xi) : \tau > 0, \xi \in \mathbb{R}\}.$$

Moreover, we identify (38) with piecewise constant functions on Ω ,

$$Q_\varepsilon(\varepsilon t, \varepsilon j + \eta) = Q_j(t) \quad \text{for every } t \geq 0, j \in \mathbb{Z}, |\eta| \leq \frac{1}{2}. \quad (39)$$

By assumption, we have $(Q_\varepsilon)_{0 < \varepsilon \leq 1} \subset L^\infty(\Omega; K)$ for some ball $K \subset \mathbb{R}^2$, and Theorem 1 provides at least one subsequence that converges to some limit measure $\mu \in YM(\Omega; K)$. Moreover, for each atomistic observable ψ we can compute the corresponding thermodynamic field via

$$\langle \psi(r, v) \rangle(\tau, \xi) = \int_{\mathbb{R}^2} \psi(r, v) \mu(\tau, \xi, dr dv).$$

We are now able to state and prove the main result on the thermodynamic limit of forced NN chains. It is a direct consequence of the discrete conservation laws derived from (1), the notion of Young-measure convergence, and the properties of distributional derivatives.

Theorem 2 (Macroscopic conservation laws for NN chains). *The thermodynamic fields of each Young measure limit μ of (1) satisfy the conservation laws (5) within the following domains in the sense of distributions: The laws for mass (5)₁ and momentum (5)₂ hold for Ω . The conservation of energy (5)₃ holds for Ω if $\zeta \equiv 0$, and otherwise for $\tilde{\Omega} := \Omega \setminus \{\xi = 0\}$.*

Proof. Within this proof we write $Q_\varepsilon(\tau, \xi) = (r_\varepsilon(\tau, \xi), v_\varepsilon(\tau, \xi))$. The equation of motion (1), combined with the scaling rules (4) and (39), implies the following discrete conservation laws

$$\partial_\tau r_\varepsilon - \nabla_{+\varepsilon} v_\varepsilon = 0, \quad (40)$$

$$\partial_\tau v_\varepsilon - \nabla_{-\varepsilon} \Phi'(r_\varepsilon) = \zeta(\tau/\varepsilon) \chi_\varepsilon(\xi), \quad (41)$$

$$\partial_\tau \left(\frac{1}{2} v_\varepsilon^2 + \Phi(r_\varepsilon) - \varepsilon \nabla_{-\varepsilon} \Phi(r_\varepsilon) \right) - \nabla_{-\varepsilon} (v_\varepsilon \Phi'(r_\varepsilon)) = \zeta(\tau/\varepsilon) v_0(\tau/\varepsilon) \chi_\varepsilon(\xi) \quad (42)$$

for all $\tau > 0$ and almost all $\xi \in \mathbb{R}$, where the discrete differential operators $\nabla_{\pm\varepsilon}$ and the scaled cut off function χ_ε are given by

$$(\nabla_{\pm\varepsilon} f)(\tau, \xi) = \frac{\pm f(\tau, \xi \pm \varepsilon) \mp f(\tau, \xi)}{\varepsilon}, \quad \chi_\varepsilon(\xi) = \frac{\chi_{\{|\xi| \leq \varepsilon/2\}}(\xi)}{\varepsilon}.$$

We now multiply (40) with a test function $\phi \in C_c^\infty(\Omega)$ and integrate with respect to both τ and ξ . Using integration by parts and expansions with respect to ε we then find

$$\int_{\Omega} r_\varepsilon \partial_\tau \phi - v_\varepsilon \partial_\xi \phi d\tau d\xi = O(\varepsilon),$$

so the limit $\varepsilon \rightarrow 0$ provides (5)₁ in the sense of distributions, see (37). Similarly, and using that (15) implies

$$\int_{\Omega} \zeta(\tau/\varepsilon) \chi_{\varepsilon}(\xi) \phi(\tau, \xi) \, d\tau d\xi = \varepsilon \int_0^{\infty} \zeta(t) \phi(\varepsilon t, 0) \, dt + O(\varepsilon) = O(\varepsilon),$$

we derive (5)₂ from (41). Finally, the assertions about the energy conservation follow from (42), where for $\zeta \neq 0$ we assume that all test functions ϕ are compactly supported in $\tilde{\Omega}$. \square

Since the energy is conserved in $\tilde{\Omega}$ we can balance the energy in the whole domain Ω via (16).

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